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Discrete-time moment closure models for epidemic spreading in populations of interacting individuals

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HIGHLIGHTS

- Derivation of a novel set of 'discrete-time moment equations' at the level of individual nodes and pairs of nodes.
- Introduction of appropriate approximations of the joint probabilities appearing in the 'discrete-time moment equations' to close them.
- Formulation of two types of model: one assuming statistical independence at the level of individuals and one at the level of pairs.
- Derivation of a model at the level of the population which captures the behavior of epidemics on homogeneous random networks.
- Validation of the proposed models through numerical simulation over different network topologies.

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ABSTRACT

Understanding the dynamics of spread of infectious diseases between individuals is essential for forecasting the evolution of an epidemic outbreak or for defining intervention policies. The problem is addressed by many approaches including stochastic and deterministic models formulated at diverse scales (individuals, populations) and different levels of detail. Here we consider discrete-time SIR (susceptible–infectious–removed) dynamics propagated on contact networks. We derive a novel set of 'discrete-time moment equations' for the probability of the system states at the level of individual nodes and pairs of nodes. These equations form a set which we close by introducing appropriate approximations of the joint probabilities appearing in them. For the example case of SIR processes, we formulate two types of model, one assuming statistical independence at the level of individuals and one at the level of pairs. From the pair-based model we then derive a model at the level of the population which captures the behavior of epidemics on homogeneous random networks. With respect to their continuous-time counterparts, the models include a larger number of possible transitions from one state to another and joint probabilities with a larger number of individuals. The approach is validated through numerical simulation over different network topologies.

1. Introduction

Epidemic modeling is a continuously evolving field that is increasingly important for understanding the spread of infectious diseases, investigating outbreak scenarios, and identifying prevention and control policies (Pastor-Satorras et al., 2015; Fu et al., 2013). For example, mathematical models of the 2014 West Africa Ebola outbreak have provided valuable quantitative analysis for assessing the risk of international virus diffusion, the impact of travel restrictions, and the effectiveness of intervention strategies (Gomes et al., 2014; Poletto et al., 2014; Merler et al., 2015).

Early models of the spread of infectious diseases were based on deterministic ordinary differential equations (Anderson et al., 1992; Heesterbeek, 2000) using the assumption of homogeneous mixing between individuals in the population (that is, any two individuals are equally likely to interact at any time, Pastor-Satorras et al., 2015), and provided a description of the epidemics at the level of the population. With the introduction of complex networks (Newman, 2003; Boccaletti et al., 2006) into epidemics models, the hypothesis of homogeneous mixing was removed by explicitly incorporating the heterogeneity of the interaction pattern among individuals (Pastor-Satorras and Vespignani, 2001; Lloyd and May, 2001). These models and the related theoretical approaches to understanding their critical properties (Moreno et al., 2002; Newman, 2002; Barthélemy et al., 2004) have been widely studied. The investigation of network-based

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approaches has led to the development of microsimulation models, able to track billions of individuals, and used to perform stochastic simulations of entire populations at the scale of single individuals, by explicitly taking into account the spatial structures and individual heterogeneity that can be inferred from the analysis of available datasets on the structure of human interactions, their mobility and contact patterns (Merler et al., 2011; Gomes et al., 2014).

In parallel to stochastic simulation methods, deterministic representations of epidemic dynamics on networks have also been developed. In scenarios where infection is treated as spreading from individual to individual via a network of contacts, pair approximation methods have proved to be a valuable extension to the classic mean-field methods. These methods have been investigated both at the population level (Matsuda et al., 1992; Keeling, 1999) and at the individual node level (Sharkey, 2008, 2011). Insights into the relationship between microscopic stochastic dynamics and mean-field descriptions are gained through the analysis of these models (Sharkey, 2008).

Although most of the mean-field or pair approximation models are based on continuous time, a few works have dealt with their discrete-time counterpart (Wang et al., 2003; Gómez et al., 2010; Valdano et al., 2015). On the other hand, stochastic discrete-time epidemic models are widely used (Pastor-Satorras et al., 2015; Frasca et al., 2006; Buscarino et al., 2008, 2014), especially in data-driven approaches where information is available at discrete sample times. Consequently, developing deterministic versions of discrete-time models may offer a relevant complementary approach. Furthermore, the dynamics of discrete-time models is typically far richer in behavior than their analogous continuous-time counterparts.

In previous works on deterministic discrete-time models, Markov chains have been employed to model SI (susceptible–infectious) or SIS (susceptible–infectious–susceptible) processes on static contact networks (Wang et al., 2003; Gómez et al., 2010), and then extended to deal with the case of temporal networks in Valdano et al. (2015). However, these works investigate epidemic processes under the assumption of stationarity and also assume the absence of correlations between individual infection probabilities. In our work, we derive the 'discrete-time moment equations' for the probability of the states of an SIR process. A novel feature of these discrete-time equations is that, unlike a standard continuous-time BBGKY-type hierarchy of moment equations, they are expressed in terms of joint probabilities whose degree is governed by the network structure itself via the degrees of individual nodes. To close these equations we introduce appropriate approximations of the joint probabilities that appear. We do this with two different assumptions on statistical independence: one at the level of individuals and one at the level of pairs. We then derive models at the level of the population from the individual-based and pair-based ones by making appropriate homogeneity assumptions (Sharkey, 2008). We validate the approach through numerical evaluation and compare the results with stochastic simulation.

2. Individual-based model

We consider an undirected network $\mathcal{G}=(\mathcal{N},\mathcal{L})$ with N nodes and L edges. Two nodes $i,j\in\mathcal{N}$ are connected only if $(i,j)\in\mathcal{L}$, and self-loops are not allowed, that is, $(i,i)\notin\mathcal{L}$.

Each node of the network represents an individual and a link is a contact between two individuals. In this framework, we consider the terms 'individuals' and 'nodes' to be synonymous. The network is also represented by its adjacency matrix G, where $G_{ij}=1$ if there is contact from individual j to individual i, and $G_{ij}=0$ otherwise.

We focus on the discrete-time SIR model, where each node/individual may assume one of the three possible states denoted as S, I, and R. A susceptible individual may become infected if contacted by an infectious individual with a probability given by T_{ij}. In the case where the transmission rate across each link per unit time is the same and equal to τ, then $T_{ij}=\tau G_{ij}$. An infected individual recovers from the disease with probability γ per unit time.

We denote the probability that the i-th individual is in the susceptible, infectious or recovered state at time t by $\langle S_i\rangle_t$, $\langle I_i\rangle_t$ and $\langle R_i\rangle_t$, respectively. Additionally, for convenience we also introduce the uninfected state U as a state in which the agent is either susceptible or recovered, and denote the probability that the i-th individual is in this state by $\langle U_i\rangle_t$ (by definition $\langle U_i\rangle_t=\langle S_i\rangle_t+\langle R_i\rangle_t$). The discrete-time equations governing the evolution of the state probabilities are:

$$\begin{aligned}\langle S_i\rangle_{t+1}&=\langle S_i\rangle_t-\Pi_{S_i\to I_i}\\ \langle I_i\rangle_{t+1}&=\langle I_i\rangle_t+\Pi_{S_i\to I_i}-\Pi_{I_i\to R_i}\end{aligned}\tag{1}$$

where $\Pi_{S_i\to I_i}$ represents the probability that the i-th individual in the state S becomes infectious and $\Pi_{I_i\to R_i}$ the probability that the i-th individual in the state I recovers from the disease.

To develop expressions for these terms, we need to introduce the subset $\mathcal{N}_i\subseteq\mathcal{N}$ containing the node i and all its first neighbors, and the subset $\mathcal{L}_i\subseteq\mathcal{L}$ containing all of the arcs connecting i to one of its first neighbors. Let us assume that the cardinality of $\mathcal{N}_i$ is m, so in addition to i there are another $m-1$ elements in $\mathcal{N}_i$. To keep the notation simple, let us define a new labelling of the nodes in $\mathcal{N}_i$ such that $J_1=i$ and the other nodes are $J_2,J_3,J_4,\ldots,J_m$. With these definitions, the probability $\Pi_{S_i\to I_i}$ reads:

$$\begin{aligned}\Pi_{S_i\to I_i}=&\langle S_iI_{J_2}U_{J_3}U_{J_4}\ldots U_{J_m}\rangle_t[1-(1-T_{iJ_2})]\\ &+\langle S_iU_{J_2}I_{J_3}U_{J_4}\ldots U_{J_m}\rangle_t[1-(1-T_{iJ_3})]+\cdots\\ &+\langle S_iU_{J_2}U_{J_3}U_{J_4}\ldots I_{J_m}\rangle_t[1-(1-T_{iJ_m})]\\ &+\langle S_iI_{J_2}I_{J_3}U_{J_4}\ldots U_{J_m}\rangle_t[1-(1-T_{iJ_2})(1-T_{iJ_3})]\\ &+\langle S_iI_{J_2}U_{J_3}I_{J_4}\ldots U_{J_m}\rangle_t[1-(1-T_{iJ_2})(1-T_{iJ_4})]+\cdots\\ &+\langle S_iI_{J_2}I_{J_3}\ldots I_{J_m}\rangle_t\left[1-\prod_{h=2}^{m}(1-T_{iJ_h})\right]\end{aligned}\tag{2}$$

where $i\in\{1,2,\ldots,N\}$. We note that $\Pi_{S_i\to I_i}$ is a function of the probabilities of the different possible states of the nodes of $\mathcal{N}_i\backslash\{i\}$ given that node i itself is susceptible. Each term on the right-hand side of (2) expresses the joint probability of the states of m individuals multiplied by the probability that, given that state, i gets infected over the next time step. For example, the term $\langle S_iI_{J_2}U_{J_3}\ldots U_{J_m}\rangle_t$ represents the probability that individual i is susceptible, J_2 is infected, and all the others are uninfected. Under this condition, i can be infected only through contact with J_2. In fact, the term $(1-T_{iJ_2})$ represents the probability that i does not get infected through the link with J_2 and $[1-(1-T_{iJ_2})]$ the probability that it does. Similarly, when contacts with more than one infected individuals are possible, for instance, if $\langle S_iI_{J_2}I_{J_3}U_{J_4}\ldots U_{J_m}\rangle_t\neq 0$, then $(1-T_{iJ_2})(1-T_{iJ_3})$ is the probability that i does not get infected through the link with J_2 or through the link with J_3, and $[1-(1-T_{iJ_2})(1-T_{iJ_3})]$ is the probability that it does.

By contrast the recovery probability $\Pi_{I_i\to R_i}$ does not depend on the state of the neighbors, and is expressed by:

$$\Pi_{I_i\to R_i}=\gamma\langle I_i\rangle_t.\tag{3}$$

Eq. (1) is exact, but not closed. We propose to close it either at the level of individuals or at the level of pairs. The first case is dealt with in this section, while the second one is discussed in Section 3. In the first case, we assume statistical independence at the level of the individual probabilities; that is, we approximate the m-node state (or m-state) probability as:

$$\langle A_iB_{J_2}C_{J_3}D_{J_4}\ldots M_{J_m}\rangle\approx\langle A_i\rangle\langle B_{J_2}\rangle\langle C_{J_3}\rangle\langle D_{J_4}\rangle\ldots\langle M_{J_m}\rangle\tag{4}$$

where $A_i, B_{J_2}, C_{J_3}, D_{J_4}, \ldots, M_{J_m}$ denote the state of nodes $i, J_2, J_3, J_4, \ldots, J_m$, respectively. Under this assumption, $\Pi_{S_i \to I_i}$ may be approximated as:

$$\Pi_{S_i \to I_i} \approx \langle S_i \rangle_t \left[1 - \prod_{h=2}^{m} (1 - T_{ij_h} \langle I_{J_h} \rangle_t) \right]. \tag{5}$$

We can show this by writing the right-hand side as:

$$\langle S_i \rangle_t \left[1 - \prod_{h=2}^{m} (1 - T_{ij_h} \langle I_{J_h} \rangle_t) \right] = \langle S_i \rangle_t \left[\sum_h T_{ij_h} \langle I_{J_h} \rangle_t - \sum_{h,l} T_{ij_h} T_{ij_l} \langle I_{J_h} \rangle_t \langle I_{J_l} \rangle_t + \cdots - (-1)^m \prod_h T_{ij_h} \langle I_{J_h} \rangle_t \right] \tag{6}$$

where all the sums and products are from $h=2$ to $h=m$.

Similarly, Eq. (2) may be rewritten by first approximating the term $\langle S_i I_{J_2} I_{J_3} \ldots I_{J_m} \rangle_t [1 - \prod_{h=2}^{m} (1 - T_{ij_h})]$ as:

$$\langle S_i I_{J_2} I_{J_3} \ldots I_{J_m} \rangle_t \left[1 - \prod_{h=2}^{m} (1 - T_{ij_h}) \right] \approx \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \ldots \langle I_{J_m} \rangle_t \left[\sum_h T_{ij_h} - \sum_{h,l} T_{ij_h} T_{ij_l} + \cdots - (-1)^m \prod_h T_{ij_h} \right]. \tag{7}$$

By suitably regrouping the terms in the right-hand side of Eq. (2) under the assumption of statistical independence (Eq. (4)) and taking into account that $\langle U_{J_h} \rangle_t + \langle I_{J_h} \rangle_t = 1, \forall J_h$, we obtain:

$$\begin{aligned}
\Pi_{S_i \to I_i} \approx\ & \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle U_{J_3} \rangle_t \ldots \langle U_{J_m} \rangle_t T_{ij_2} + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \ldots \langle U_{J_m} \rangle_t T_{ij_2} + \cdots \\
& + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle U_{J_3} \rangle_t \ldots \langle I_{J_m} \rangle_t T_{ij_2} + \cdots + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \ldots \langle I_{J_m} \rangle_t T_{ij_2} + \cdots \\
& + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \langle U_{J_4} \rangle_t \ldots \langle U_{J_m} \rangle_t T_{ij_2} T_{ij_3} + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \langle I_{J_4} \rangle_t \ldots \langle U_{J_m} \rangle_t T_{ij_2} T_{ij_3} \\
& + \cdots + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \langle U_{J_4} \rangle_t \ldots \langle I_{J_m} \rangle_t T_{ij_2} T_{ij_3} + \cdots \\
& + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \langle I_{J_4} \rangle_t \ldots \langle I_{J_m} \rangle_t T_{ij_2} T_{ij_3} + \cdots \\
& - (-1)^m \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \ldots \langle I_{J_m} \rangle_t T_{ij_2} T_{ij_3} \ldots T_{ij_m} = \langle S_i \rangle_t \langle I_{J_2} \rangle_t T_{ij_2} + \cdots \\
& + \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t T_{ij_2} T_{ij_3} + \cdots - (-1)^m \langle S_i \rangle_t \langle I_{J_2} \rangle_t \langle I_{J_3} \rangle_t \ldots \langle I_{J_m} \rangle_t T_{ij_2} T_{ij_3} \ldots T_{ij_m} \\
=\ & \langle S_i \rangle_t \left[\sum_h T_{ij_h} \langle I_{J_h} \rangle_t - \sum_{h,l} T_{ij_h} T_{ij_l} \langle I_{J_h} \rangle_t \langle I_{J_l} \rangle_t + \ldots - (-1)^m \prod_h T_{ij_h} \langle I_{J_h} \rangle_t \right]
\end{aligned} \tag{8}$$

which is the same as Eq. (6), thereby obtaining Eq. (5).

We note that, under the hypothesis of statistical independence, the expression for the infection term (5) is analogous to that found in Wang et al. (2003) and Gómez et al. (2010) for stationary probabilities in an SI/SIS process.

3. Pair-based model

In this section, we write the 'moment equations' for a discrete-time SIR process at the level of pairs. If we inspect the dynamics of the state probabilities in an SIR process, as in Eqs. (1), we recognize that recovery happens at the level of the individual who recovers from the disease with a probability independent from the states of the other individuals, while infection takes place with a probability that also depends on the states of the contacts of the individual. The different nature of the two processes is mirrored in the expressions for the transition probabilities $\Pi_{I_i \to R_i}$ and $\Pi_{S_i \to I_i}$, the first being only a function of $\langle I_i \rangle_t$ and the second of joint probabilities of the states of m individuals. To close the system, an approximation is needed for these joint probabilities, and the accuracy of the model depends on the validity of this approximation. In Section 2, we assumed statistical independence at the level of individuals in order to generate a closure. Here we shall avoid this assumption and instead consider statistical independence at the level of pairs. This still results in a significant dimensional reduction of the system while incorporating a more detailed description than the individual-based model. With this approach we would expect to derive a more accurate model due to the incorporation of pairwise correlations; indeed, studies focusing on the continuous-time case (Keeling, 1999; Sharkey, 2008; House and Keeling, 2010) have provided evidence of an improved description.

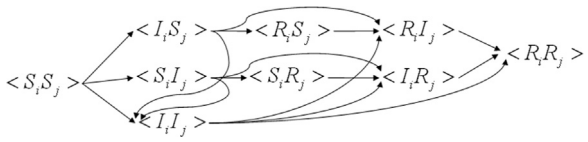

Fig. 1. Possible states and transitions in the pair-based model for a SIR process. Note that, for example, $\langle I_i S_j \rangle = \langle S_j I_i \rangle$ when comparing with Eq. (9).

To provide a description at the level of pairs, we need dynamic variables representing pair probabilities. In particular, for an SIR process the following variables have to be taken into account: $\langle S_i S_j \rangle_t$, $\langle S_i I_j \rangle_t$, $\langle I_i I_j \rangle_t$, $\langle R_i S_j \rangle_t$, $\langle R_i I_j \rangle_t$, and $\langle R_i R_j \rangle_t$ for each link of the network; that is, $(i,j) \in \mathcal{L}$. The pair variables are shown in Fig. 1 along with the possible transitions among them. Based on this diagram, we derive the complete moment equations for the pair dynamics in the SIR model as:

$$\begin{aligned}
\langle S_i S_j \rangle_{t+1} &= \langle S_i S_j \rangle_t - \Pi_{S_i S_j \to I_i S_j} - \Pi_{S_i S_j \to S_i I_j} - \Pi_{S_i S_j \to I_i I_j} \\
\langle S_i I_j \rangle_{t+1} &= \langle S_i I_j \rangle_t + \Pi_{S_i S_j \to S_i I_j} - \Pi_{S_i I_j \to S_i R_j} - \Pi_{S_i I_j \to I_i I_j} - \Pi_{S_i I_j \to I_i R_j} \\
\langle I_i I_j \rangle_{t+1} &= \langle I_i I_j \rangle_t + \Pi_{S_i S_j \to I_i I_j} + \Pi_{S_i I_j \to I_i I_j} + \Pi_{I_i S_j \to I_i I_j} - \Pi_{I_i I_j \to R_i I_j} \\
&\quad - \Pi_{I_i I_j \to I_i R_j} - \Pi_{I_i I_j \to R_i R_j} \\
\langle R_i S_j \rangle_{t+1} &= \langle R_i S_j \rangle_t + \Pi_{I_i S_j \to R_i S_j} - \Pi_{R_i S_j \to R_i I_j} \\
\langle R_i I_j \rangle_{t+1} &= \langle R_i I_j \rangle_t + \Pi_{R_i S_j \to R_i I_j} + \Pi_{I_i I_j \to R_i I_j} + \Pi_{I_i S_j \to R_i I_j} - \Pi_{R_i I_j \to R_i R_j} \\
\langle R_i R_j \rangle_{t+1} &= \langle R_i R_j \rangle_t + \Pi_{I_i R_j \to R_i R_j} + \Pi_{R_i I_j \to R_i R_j} + \Pi_{I_i I_j \to R_i R_j}
\end{aligned} \tag{9}$$

where $(i,j) \in \mathcal{L}$ and the terms $\Pi_{A_i B_j \to A_i' B_j'}$ represent the transition from the (A_i, B_j) state to the (A_i', B_j') state. To form expressions for these terms, we introduce two subsets: $\mathcal{N}_{(i,j)} \subseteq \mathcal{N}$ and $\mathcal{S}_{(i,j)} \subseteq \mathcal{L}$. The subset $\mathcal{N}_{(i,j)} \subseteq \mathcal{N}$ contains all vertices which are first neighbors of node i or j or of both; that is $\mathcal{N}_{(i,j)} = \{h : (i,h) \in \mathcal{L} \text{ or } (h,j) \in \mathcal{L}\}$. Let us denote the cardinality of $\mathcal{N}_{(i,j)}$ by m, so that beyond i and j there are another $m-2$ elements in $\mathcal{N}_{(i,j)}$. We label the nodes according to a new index $J_1, J_2, \ldots, J_m$ such that $J_1 = i, J_2 = j$ and $J_3, \ldots, J_m$ are the other nodes in $\mathcal{N}_{(i,j)}$. The subgraph $S_{(i,j)}$ contains all the edges of $\mathcal{L}$ among the nodes in $\mathcal{N}_{(i,j)}$.

Here, we give the expression for $\Pi_{S_i S_j \to I_i S_j}$, while the other terms are detailed in Appendix A. Given the above definitions, $\Pi_{S_i S_j \to I_i S_j}$ reads:

$$\begin{aligned}
\Pi_{S_i S_j \to I_i S_j} =\ & \langle S_i S_j I_{J_3} U_{J_4} U_{J_5} \ldots U_{J_m} \rangle_t [1 - (1 - T_{ij_3})][1 - T_{jj_3}] \\
& + \langle S_i S_j U_{J_3} I_{J_4} U_{J_5} \ldots U_{J_m} \rangle_t [1 - (1 - T_{ij_4})][1 - T_{jj_4}] + \cdots \\
& + \langle S_i S_j I_{J_3} I_{J_4} U_{J_5} \ldots U_{J_m} \rangle_t [1 - (1 - T_{ij_3})(1 - T_{ij_4})][(1 - T_{jj_3})(1 - T_{jj_4})] \\
& + \langle S_i S_j U_{J_3} I_{J_4} I_{J_5} \ldots U_{J_m} \rangle_t [1 - (1 - T_{ij_4})(1 - T_{ij_5})][(1 - T_{jj_4})(1 - T_{jj_5})] + \cdots \\
& + \langle S_i S_j I_{J_3} I_{J_4} I_{J_5} \ldots U_{J_m} \rangle_t [1 - (1 - T_{ij_3})(1 - T_{ij_4})(1 - T_{ij_5})][(1 - T_{jj_3})(1 - T_{jj_4}) \\
& \times (1 - T_{jj_5})] + \cdots + \langle S_i S_j I_{J_3} I_{J_4} I_{J_5} \ldots I_{J_m} \rangle_t \left[1 - \prod_{h=3}^{m} (1 - T_{ij_h}) \right] \left[\prod_{h=3}^{m} (1 - T_{jj_h}) \right].
\end{aligned} \tag{10}$$

Note that since the transition is from $S_i S_j$ to $I_i S_j$, node i has to be infected while at the same time agent j has not to be infected, so that, for instance, when only J_3 is in the infective state, the probability $\langle S_i S_j I_{J_3} U_{J_4} U_{J_5} \ldots U_{J_m} \rangle_t$ has to be multiplied by the probability that J_3 infects i; that is, $[1 - (1 - T_{ij_3})]$, and by the probability that J_3 does not infect j, that is, $[1 - T_{jj_3}]$. It is not important to distinguish a priori if J_3 is a neighbor of i or of j because if there is no contact between J_3 and j (or i), then $T_{jj_3} = 0$ ($T_{ij_3} = 0$).

4. Closure for the pair-based model

The selection of the closure for pair-based models is a critical step. In a recent paper (Pellis et al., 2015) the quality of several closures is investigated in relation to their application to network motifs as well as to larger topologies. We refer the reader to that paper for a detailed discussion and here observe that none of the closure approximations outperform the others on all of the possible case studies. The analysis by Pellis et al. (2015) is developed in the context of continuous-time models, where only triple probabilities appear in the master equations. Here the problem is complicated by the presence of m-tuple probabilities in Eqs. (9) (see Eq. (10) and Appendix A for the terms in this equation). This requires the use of a new closure, extending the previous approaches to m-state probabilities.

Let us first consider the requirements for our closure approximation. To illustrate this, we consider a closed triangle made of three nodes (labeled 1, 2 and 3), and calculate the increment of the probability of being infected for node 2; that is $\Delta\langle I_2\rangle = \langle I_2\rangle_{t+1} - \langle I_2\rangle_t$. From the expression for the infectious probability for individual nodes (Eqs. (1) and (2)) we derive:

$$\Delta\langle I_2\rangle = \Pi_{S_2\to I_2} - \Pi_{I_2\to R_2} = (\langle S_2I_1S_3\rangle_t + \langle S_2I_1R_3\rangle_t + \langle S_2S_1I_3\rangle_t + \langle S_2R_1I_3\rangle_t)\tau + \langle S_2I_1I_3\rangle_t(1-(1-\tau)^2) - \langle I_2\rangle_t\gamma. \quad (11)$$

On the other hand, from the equations at the pair level (9) we get:

$$\begin{aligned}\Delta\langle I_2\rangle &= \langle S_1I_2\rangle_{t+1} + \langle I_1I_2\rangle_{t+1} + \langle R_1I_2\rangle_{t+1} - \langle S_1I_2\rangle_t - \langle I_1I_2\rangle_t - \langle R_1I_2\rangle_t \\ &= (\langle S_1S_2I_3\rangle_t + \langle I_1S_2S_3\rangle_t + \langle I_1S_2R_3\rangle_t + \langle R_1S_2I_3\rangle_t)\tau \\ &\quad + \langle I_1S_2I_3\rangle_t(1-(1-\tau)^2) - (\langle S_1I_2S_3\rangle_t + \langle S_1I_2R_3\rangle_t + \langle S_1I_2I_3\rangle_t)\gamma \\ &\quad - \langle I_1I_2\rangle_t\gamma - \langle R_1I_2\rangle_t\gamma. \end{aligned} \quad (12)$$

Clearly, the two expressions (11) and (12) must be equivalent. However, to close the system at the level of pairs we need to approximate triplet probabilities (and higher-order joint probabilities) in terms of pair and singlet probabilities. In doing this, we risk making the two expressions inconsistent. While we could permit this, designing a closure with this consistency is arguably aesthetically preferable (House and Keeling, 2010; Rogers, 2011).

Let us focus on triplets and suppose that we approximate $\langle A_iB_jC_k\rangle$ by a function of the pair and individual states; that is:

$$\langle A_iB_jC_k\rangle \approx F(\langle A_iB_j\rangle, \langle B_jC_k\rangle, \langle A_iC_k\rangle, \langle A_i\rangle, \langle B_j\rangle, \langle C_k\rangle) \quad (13)$$

where we have dropped the time subscript. For the purposes of brevity, let us also indicate $F(\langle A_iB_j\rangle, \langle B_jC_k\rangle, \langle A_iC_k\rangle, \langle A_i\rangle, \langle B_j\rangle, \langle C_k\rangle)$ by $F(A_iB_jC_k)$ in what follows.

Now, the two expressions (11) and (12) coincide if the following conditions on the approximating function hold:

$$F(S_1I_2S_3) + F(S_1I_2I_3) + F(S_1I_2R_3) = \langle S_1I_2\rangle \quad (14)$$

and

$$F(A_1B_2C_3) = F(B_2A_1C_3). \quad (15)$$

In particular, the first one indicates that the closure agrees with the marginals it is constructed from; that is $\sum_{C_3} F(A_1B_2C_3) = \langle A_1B_2\rangle$ (where the summation is over all possible states for node 3; $C_3 \in \{S_3, I_3, R_3\}$). The second one indicates that the closure is symmetric with respect to its first two arguments.

In the more general case, when m-state probabilities have to be approximated on arbitrary graphs, we want the closure to be consistent with its marginals:

$$\sum_{C_3, D_4, \ldots, M_m} F(A_iB_jC_3D_4\ldots M_m) = \langle A_iB_j\rangle. \quad (16)$$

The other sufficient condition is that it is symmetric in all of its arguments. Note that this is not a necessary condition as the specific example illustrated.

The closure introduced in this paper builds on the existing ones for triplets. In particular, in the literature on population level epidemiological models, a common closure approximation in terms of pairs approximates $\langle A_iB_jC_k\rangle$ by

$$\langle A_iB_jC_k\rangle \approx \frac{\langle A_iB_j\rangle\langle A_iC_k\rangle\langle B_jC_k\rangle}{\langle A_i\rangle\langle B_j\rangle\langle C_k\rangle} \quad (17)$$

if i and k are connected (closed triplet Kirkwood, 1935; Keeling, 1999), or by

$$\langle A_iB_jC_k\rangle \approx \frac{\langle A_iB_j\rangle\langle B_jC_k\rangle}{\langle B_j\rangle} \quad (18)$$

if i and k are not connected. Both of these closures can be subsumed within a more general framework for approximating m-states (Sharkey and Wilkinson, 2015, Eq. (14)):

$$\langle A_iB_jC_{J_3}D_{J_4}\ldots M_{J_m}\rangle \approx y(S_{(i,j)}, A_i, B_j, C_{J_3}, D_{J_4}, \ldots, M_{J_m}) \quad (19)$$

where

$$y(S_{(i,j)}, A_i, B_j, C_{J_3}, D_{J_4}, \ldots, M_{J_m}) = \frac{\prod_{(h,l)\in S_{(i,j)}}\langle H_{J_h}L_{J_l}\rangle}{\langle A_i\rangle^{k_i^S-1}\langle B_j\rangle^{k_j^S-1}\langle C_{J_3}\rangle^{k_{J_3}^S-1}\ldots\langle M_{J_m}\rangle^{k_{J_m}^S-1}} \quad (20)$$

and where $k_{J_h}^S$ is the degree of node J_h in the subgraph $S_{(i,j)}$.

However, we observe that $y(S_{(i,j)}, A_i, B_j, C_{J_3}, D_{J_4}, \ldots, M_{J_m})$ does not satisfy the property (16). For this reason, following House and Keeling (2010) and Rogers (2011) we introduce the following 'improved pairwise closure' approximation:

$$Y(S_{(i,j)}, A_i, B_j, C_{J_3}, \ldots, M_{J_n}) = \langle A_iB_j\rangle \frac{y(\bar{S}_{(i,j)}, A_i, B_j, C_{J_3}, \ldots, M_{J_m})}{\sum_{C_{J_3}, D_{J_4}, \ldots, M_{J_m}} y(\bar{S}_{(i,j)}, A_i, B_j, C_{J_3}, \ldots, M_{J_m})} \quad (21)$$

where $\bar{S}_{(i,j)} = S_{(i,j)} \setminus (i,j)$.

It is easy to verify that $Y(S_{(i,j)}, A_i, B_j, C_{J_3}, \ldots, M_{J_n})$ satisfies the condition (16). Furthermore, if there are no edges between the nodes $J_3, J_4, \ldots, J_m$ in $S_{(i,j)}$, then $Y(S_{(i,j)}, A_i, B_j, C_{J_3}, \ldots, M_{J_n})$ coincides with $y(S_{(i,j)}, A_i, B_j, C_{J_3}, \ldots, M_{J_n})$.

5. Numerical simulations

In this section, the behavior of the individual-based and pair-based discrete-time moment closure models are compared with stochastic simulations on static, undirected network topologies. As an example of an arbitrary, random topology, we consider an Erdös–Renyi (ER) undirected network with $N=100$ nodes. The network is constructed by connecting each pair of nodes with a probability $p=0.03$ (and checking that the final network is strongly connected), which leads to an average node degree of approximately $\langle k\rangle \approx pN = 3$. Epidemic spreading on this network was simulated by initiating the same individual in the infective state for the individual-based and pair-based models, and for stochastic simulation of the underlying stochastic SIR model. Simulations are initiated from a single infective because this is where discrepancies are expected to be greatest (Sharkey, 2011). For each set of parameters, 1000 stochastic simulations were run. Fig. 2 illustrates the time series of the number of infective individuals $I(t)$ generated by the two deterministic models and by stochastic simulations for $\tau = 0.3$ and $\gamma = 0.15$. For the deterministic models, we obtain the approximate expected number of infective by using the fact that, in the absence of approximation, the expected number of infective is $I(t) = \sum_i \langle I_i\rangle_t$. For stochastic simulations, the average number of infective individuals over the realizations of the stochastic process is shown.

The pair-based model offers a prediction which is in good agreement with the average behavior of the stochastic simulations

of the epidemics, while the individual-based model significantly overestimates the number of infective individuals. In general, the performance of the deterministic models depends on the given values used for simulating the epidemic process; that is, of the per-contact infection and recovery probabilities. This is clearly visible in Fig. 3, showing the final size of the recovered population normalized by the number of individuals, R_∞/N, as a function of τ for fixed γ. For both low and large values of τ, the final size of the recovered population is accurately estimated by both the individual-based and pair-based models, while the largest errors are observed for intermediate values of τ, where the variability of the stochastic simulations is greater and the phenomenon of epidemic fade-out is still significant. In this region of parameter space, the pair-based model significantly outperforms the individual-based one. We also note that the pair-based model captures the transition in Fig. 3 suggesting that it makes a reasonably accurate estimation of the epidemic threshold, while the error in the individual-based one is larger.

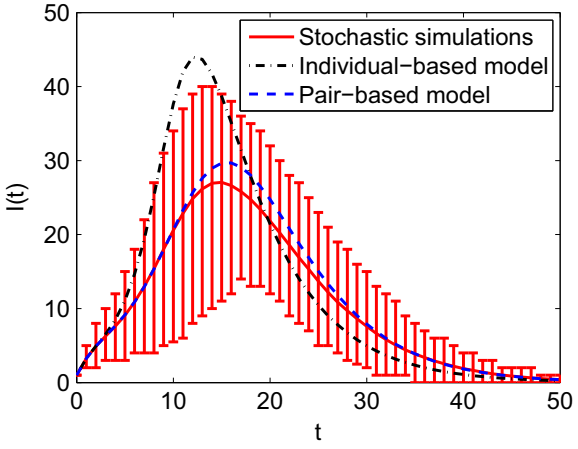

Fig. 2. Comparison between stochastic simulations (averaged over 1000 runs), individual-based model and pair-based model for a ER network with $N=100$, $p=0.03$, $\tau=0.3$, $\gamma=0.15$. Error bars indicate the 10th and 90th percentiles of stochastic simulations.

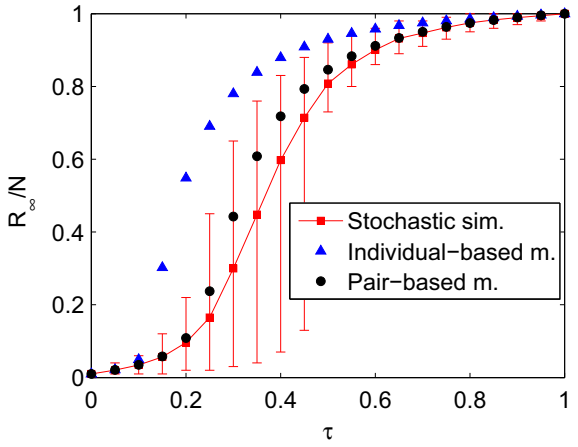

Fig. 3. The normalized size of the recovered population, R_∞/N, is shown as a function of τ for fixed γ ($\gamma=0.4$) for an ER network with $N=100$ nodes. Error bars indicate the 10th and 90th percentiles of stochastic simulations.

We now discuss the performance of the deterministic models on two other topologies. The first of these is a tree with $N=100$ nodes and an average node degree equal to $\langle k\rangle\approx 3$. The comparison between the three models is illustrated in Fig. 4(a) and clearly shows how the pair-based model accurately predicts the average evolution of the stochastic simulations, while the individual-based model fails to do this. This finding is in line with the results of Sharkey (2008), Pellis et al. (2015) and Sharkey et al. (2015). However, while pair-based closures for continuous-time SIR epidemic models on trees are exact (Sharkey and Wilkinson, 2015; Sharkey et al., 2015), the closure expression (21) is not since it can have infectious nodes on the denominator; this explains the small discrepancy between the stochastic simulations and the prediction offered by the pair-based model that can be observed in Fig. 4(a). Note that this is also true of expression (20) which is equivalent to (21) on a tree.

The other structure we consider (a triangular lattice, Fig. 4(b)) represents an attempt at a worst-case scenario where many cycles of all sizes are present. Fig. 4(b) shows a significant difference between the trend of the stochastic simulations and that of the deterministic prediction. Although the individual-based model could be argued to be a better qualitative representation of the time evolution with regard to this figure, the pair-based model gives a better representation of the initial phases of the infectious time series. Furthermore, it still performs much better in terms of predicting the final epidemic size; in fact, we have found $R_\infty/N=0.9730$ on average for the stochastic simulations, $R_\infty/N=0.9995$ for the individual-based model, and $R_\infty/N=0.9708$ for the pair-based model.

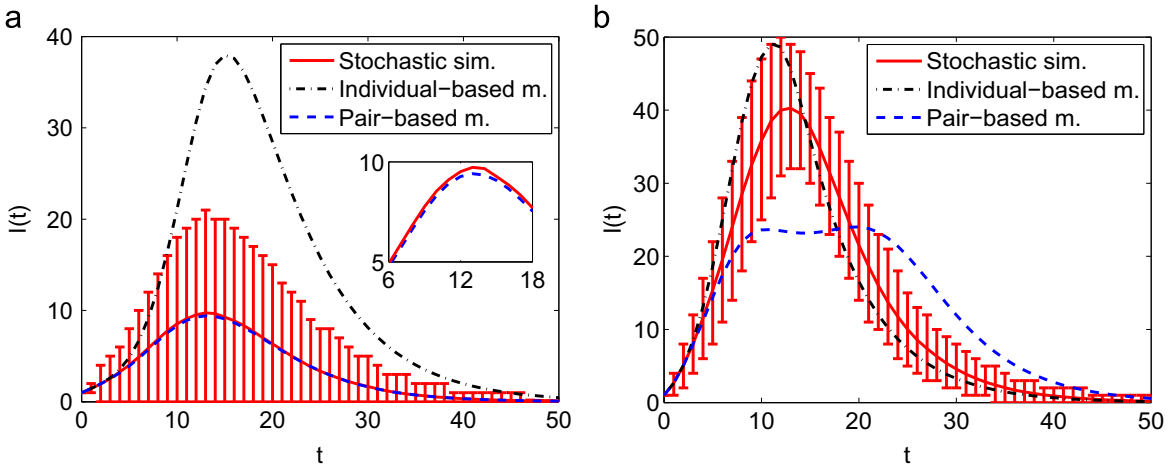

Fig. 4. Comparison between stochastic simulations (averaged over 1000 runs), individual-based model and pair-based model for two network topologies with $N=100$, $\tau=0.3$, $\gamma=0.15$: (a) a tree network with $k=3$; (b) a triangular lattice. Error bars indicate the 10th and 90th percentiles of stochastic simulations. The inset in panel (a) is a magnification showing the small discrepancy between pair-based model and stochastic simulations in the tree network.

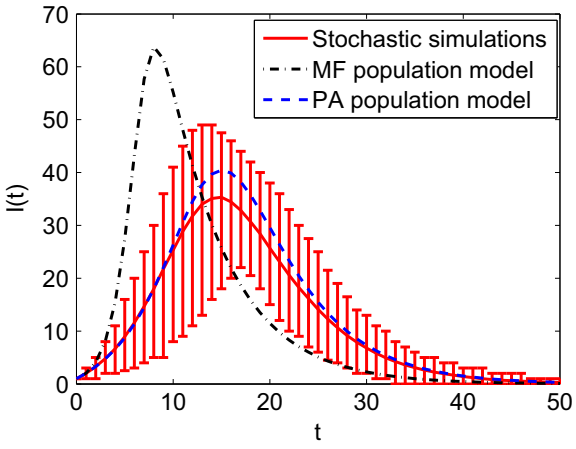

Fig. 5. Comparison between stochastic simulations (averaged over 1000 runs) and prediction offered by the MF and PA population models for a k-regular random graph with $N=100$ nodes. The parameters for the epidemic have been fixed as $\tau=0.4$ and $\gamma=0.15$. Error bars indicate the 10th and 90th percentiles of stochastic simulations.

6. Population models

In this section, we derive models at the population level by starting from the individual- and pair-based models and assuming some simplifying hypotheses. In particular, we consider idealized k-regular random graphs without cycles (recognizing that, in practice, finite versions of these do not exist). We then assume homogeneity in the states of nodes and links (Sharkey, 2008):

$$\begin{aligned}\langle S_i\rangle_t &= \langle S\rangle_t = \frac{[S]_t}{N}\\ \langle I_i\rangle_t &= \langle I\rangle_t = \frac{[I]_t}{N}\\ \langle R_i\rangle_t &= \langle R\rangle_t = \frac{[R]_t}{N}\\ \langle S_iI_j\rangle_t &= \langle SI\rangle_t = \frac{[SI]_t}{Nk}\end{aligned} \tag{22}$$

where $[S]_t$, $[I]_t$, and $[R]_t$ represent the fraction of the population in the S, I or R state. We have:

$$\begin{aligned}\langle S\rangle_{t+1} &= \langle S\rangle_t - \Pi_{S_i\to I_i}\\ \langle I\rangle_{t+1} &= \langle I\rangle_t + \Pi_{S_i\to I_i} - \Pi_{I_i\to R_i}.\end{aligned} \tag{23}$$

From the individual-based model we obtain a model at the population level by applying homogeneity in the states of nodes. Specifically, we apply expressions (22) in Eq. (5). If we indicate the per time step probability of transmission across an SI link by τ, then Eq. (5) becomes:

$$\Pi_{S_i\to I_i} \approx \langle S\rangle_t[1-(1-\tau\langle I\rangle_t)^k]. \tag{24}$$

while for the recovery probability we have:

$$\Pi_{I\to R} = \gamma\langle I\rangle_t. \tag{25}$$

For reference, we shall refer to this as the mean-field (MF) population model.

For the population model derived from the pair-based model, in the following referred to as the *pair-approximation* (*PA*) *population model*, we consider again Eqs. (23) but now rewrite $\Pi_{S_i\to I_i}$ starting from Eq. (2). If we drop the subscripts in the expression of the joint probability and indicate again the per time step probability of transmission across an SI link with τ, then Eq. (2) becomes:

$$\begin{aligned}\Pi_{S\to I} = \langle \mathrm{SIUUU}\ldots U\rangle_t[1-(1-\tau)]\binom{k}{1} + \langle \mathrm{SIIUU}\ldots U\rangle_t\left[1-(1-\tau)^2\right]\binom{k}{2}\\ + \langle \mathrm{SIIIU}\ldots U\rangle_t\left[1-(1-\tau)^3\right]\binom{k}{3} + \cdots + \langle \mathrm{SIIII}\ldots I\rangle_t\left[1-(1-\tau)^k\right]\binom{k}{k}\end{aligned} \tag{26}$$

and where in this case, the recovery probability is also given by Eq. (25).

In the hypothesis of a large k-regular random network that to first approximation contains no triangular loops (in the more general case, where a significant fraction of closed triangles appears, the approach discussed in Keeling (1999) for continuous-time models can be followed), the closure discussed in Section 4 is written as:

$$\langle SI_1\ldots I_qU_{q+1}\ldots U_k\rangle = \frac{\langle SI\rangle^q\langle SU\rangle^{k-q}}{\langle S\rangle^{k-1}}. \tag{27}$$

and so

$$\Pi_{S\to I} = \sum_{q=1}^{k}\frac{\langle SI\rangle^q\langle SU\rangle^{k-q}}{\langle S\rangle^{k-1}}[1-(1-\tau)^q]\binom{k}{q} \tag{28}$$

The equations for $\langle SS\rangle$, $\langle SI\rangle$, $\langle II\rangle$, $\langle RS\rangle$, $\langle RI\rangle$ and $\langle RR\rangle$ read as:

$$\begin{aligned}\langle SS\rangle_{t+1} &= \langle SS\rangle_t - \Pi_{SS\to IS} - \Pi_{SS\to SI} - \Pi_{SS\to II}\\ \langle SI\rangle_{t+1} &= \langle SI\rangle_t + \Pi_{SS\to SI} - \Pi_{SI\to SR} - \Pi_{SI\to II} - \Pi_{SI\to IR}\\ \langle II\rangle_{t+1} &= \langle II\rangle_t + \Pi_{SS\to II} + \Pi_{SI\to II} + \Pi_{IS\to II} - \Pi_{II\to RI} - \Pi_{II\to IR} - \Pi_{II\to RR}\\ \langle RS\rangle_{t+1} &= \langle RS\rangle_t + \Pi_{IS\to RS} - \Pi_{RS\to RI}\\ \langle RI\rangle_{t+1} &= \langle RI\rangle_t + \Pi_{RS\to RI} + \Pi_{II\to RI} + \Pi_{IS\to RI} - \Pi_{RI\to RR}\\ \langle RR\rangle_{t+1} &= \langle RR\rangle_t + \Pi_{IR\to RR} + \Pi_{RI\to RR} + \Pi_{II\to RR}.\end{aligned} \tag{29}$$

By using $\Pi_{SS\to SI} = \Pi_{SS\to IS}$, $\Pi_{IS\to II} = \Pi_{SI\to II}$, $\Pi_{II\to IR} = \Pi_{II\to RI}$, $\Pi_{IS\to RS} = \Pi_{SI\to SR}$, $\Pi_{IS\to RI} = \Pi_{SI\to IR}$ and $\Pi_{IR\to RR} = \Pi_{RI\to RR}$ we can simplify this to:

$$\begin{aligned}\langle SS\rangle_{t+1} &= \langle SS\rangle_t - 2\Pi_{SS\to IS} - \Pi_{SS\to II}\\ \langle SI\rangle_{t+1} &= \langle SI\rangle_t + \Pi_{SS\to SI} - \Pi_{IS\to RS} - \Pi_{SI\to II} - \Pi_{IS\to RI}\\ \langle II\rangle_{t+1} &= \langle II\rangle_t + \Pi_{SS\to II} + 2\Pi_{SI\to II} - 2\Pi_{II\to RI} - \Pi_{II\to RR}\\ \langle RS\rangle_{t+1} &= \langle RS\rangle_t + \Pi_{IS\to RS} - \Pi_{RS\to RI}\\ \langle RI\rangle_{t+1} &= \langle RI\rangle_t + \Pi_{RS\to RI} + \Pi_{II\to RI} + \Pi_{SI\to IR} - \Pi_{RI\to RR}\\ \langle RR\rangle_{t+1} &= \langle RR\rangle_t + 2\Pi_{RI\to RR} + \Pi_{II\to RR}\end{aligned} \tag{30}$$

where

$$\begin{aligned}\Pi_{SS\to SI} &= \langle SS\rangle\sum_{q=1}^{2k-2}\frac{\langle SI\rangle^q\langle SU\rangle^{2k-2-q}}{\langle S\rangle^{2k-2}}\sum_{h=\max(0,q-k+1)}^{\min(q,k-1)}[1-(1-\tau)^{q-h}](1-\tau)^h\\ &\quad\times\binom{k-1}{h}\binom{k-1}{q-h}\\ \Pi_{SS\to II} &= \langle SS\rangle\sum_{q=1}^{2k-2}\frac{\langle SI\rangle^q\langle SU\rangle^{2k-2-q}}{\langle S\rangle^{2k-2}}\sum_{h=\max(0,q-k+1)}^{\min(q,k-1)}[1-(1-\tau)^{q-h}][1\\ &\quad-(1-\tau)^h]\binom{k-1}{h}\binom{k-1}{q-h}\\ \Pi_{IS\to RS} &= \langle SI\rangle\sum_{q=0}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}\gamma(1-\tau)^{q+1}\binom{k-1}{q}\\ \Pi_{SI\to II} &= \langle SI\rangle\sum_{q=0}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}(1-\gamma)[1-(1-\tau)^{q+1}]\binom{k-1}{q}\\ \Pi_{SI\to IR} &= \langle SI\rangle\sum_{q=0}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}\gamma[1-(1-\tau)^{q+1}]\binom{k-1}{q}\\ \Pi_{II\to RI} &= \langle II\rangle\gamma(1-\gamma)\\ \Pi_{II\to RR} &= \langle II\rangle\gamma^2\\ \Pi_{RS\to RI} &= \langle RS\rangle\sum_{q=1}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}[1-(1-\tau)^q]\binom{k-1}{q}\\ \Pi_{RI\to RR} &= \langle RI\rangle\gamma.\end{aligned} \tag{31}$$

These expressions are derived in Appendix B.

To validate the two population models, we consider a k-regular random graph with degree distribution $P(k)=\delta(k-3)$. In Fig. 5 the behavior of stochastic simulations is compared with the prediction offered by the population models. Fig. 5 clearly shows that, although not perfect, for the considered network the system behavior may be captured by a description at the level of the population based on pair-approximation. This description improves as the number of initially infected individuals is increased, thereby reducing the probability of stochastic fade-out. On the contrary, the prediction offered by the MF population model does not adequately capture the epidemic behavior.

7. Conclusions

In this work, we have derived the first and second order discrete-time moment equations for a class of SIR epidemic dynamics on networks. These equations are closed with the introduction of appropriate approximations of the joint probabilities appearing in them. While the second order pair-level equations are novel, we demonstrated that the first order equations are equivalent to discrete-time models which exist in the literature (Wang et al., 2003; Gomez et al., 2010) yielding a new perspective on these models. A significant difference with respect to the continuous-time counterpart of these models is that the number of possible transitions between the states is larger. Additionally, the order of the terms appearing in the equations for singlet states depends on the node degree rather than being at the level of pairs as in a standard BBGKY hierarchy. To close the system, we have thus introduced closure approximations for m-tuple probabilities either by assuming statistical independence at the level of individuals or at the level of pairs.

The deterministic models were compared with stochastic simulations over several contact network topologies. We found that the pair-based model is very accurate on tree networks, although, unlike its continuous-time counterpart (Sharkey et al., 2015), it is not exact. We also found that, similar to the continuous-time case, an abundance of short cycles in the network tends to increase the inaccuracy of the model. This is due to the cycles in the network breaking the statistical independence assumptions upon which the closures are based. Generally we found that the pair-based model provides a more precise prediction of the epidemic evolution than the individual-based model.

The models introduced may be helpful to gain insights into the evolution of the epidemic dynamics at the level of individuals for discrete-time processes, since they provide a deterministic description of the infection probability for each individual. They can also be used to ground the derivation of mean field models on statistical assumptions at the microscopic scale. We presented two examples of this, one where we derived a population-level model (equivalent to that discussed in Buscarino et al, 2008) starting from the individual-based model and one where we derived a population-level model starting from the pair-based model. These models are obtained via homogeneity assumptions on the individual characteristics and network structure. The pair-level model is valid for an idealized k-regular graph with no cycles (of course, in practice we could only generate approximate finite versions of such graphs).

Finally, we note that the analysis was restricted to static undirected networks. Further work should be able to adapt these models to describe epidemic processes on time-varying contact networks.

Acknowledgments

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Appendix A. Transition terms for the pair-based model

In this Appendix, the expressions for the transition terms appearing in the pair-based model (9) are derived.

Similar to $\Pi_{S_iS_j\to I_iS_j}$, the term $\Pi_{S_iS_j\to S_iI_j}$ is given by:

$$\begin{aligned}\Pi_{S_iS_j\to S_iI_j} = {}& \langle S_iS_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_3})][1-T_{ij_3}]\\ &+\langle S_iS_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_4})][1-T_{ij_4}]+\cdots\\ &+\langle S_iS_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_3})(1-T_{jJ_4})][(1-T_{ij_3})(1-T_{ij_4})]\\ &+\langle S_iS_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_4})(1-T_{jJ_5})][(1-T_{ij_4})(1-T_{ij_5})]\\ &+\cdots+\langle S_iS_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_3})(1-T_{jJ_4})(1-T_{jJ_5})][(1-T_{ij_3})\\ &\times(1-T_{ij_4})(1-T_{ij_5})]+\cdots+\langle S_iS_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t\left[1-\prod_{h=3}^{m}(1-T_{jJ_h})\right]\\ &\times\left[\prod_{h=3}^{m}(1-T_{ij_h})\right].\end{aligned}\tag{A.1}$$

To write the term $\Pi_{S_iS_j\to I_iI_j}$, we have to take into account that now both i and j have to be infected, so that:

$$\begin{aligned}\Pi_{S_iS_j\to I_iI_j} = {}& \langle S_iS_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{iJ_3})][1-(1-T_{jJ_3})]\\ &+\langle S_iS_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{iJ_4})][1-(1-T_{jJ_4})]\\ &+\cdots+\langle S_iS_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{iJ_3})(1-T_{iJ_4})][1-(1-T_{jJ_3})(1-T_{jJ_4})]\\ &+\langle S_iS_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{iJ_4})(1-T_{iJ_5})][1-(1-T_{jJ_4})(1-T_{jJ_5})]\\ &+\cdots+\langle S_iS_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{iJ_3})(1-T_{iJ_4})\\ &\times(1-T_{iJ_5})][1-(1-T_{jJ_3})(1-T_{jJ_4})(1-T_{jJ_5})]+\cdots+\langle S_iS_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t\\ &\times\left[1-\prod_{h=3}^{m}(1-T_{ij_h})\right]\left[1-\prod_{h=3}^{m}(1-T_{jJ_h})\right].\end{aligned}\tag{A.2}$$

The transition from S_iI_j to S_iR_j occurs if i is not infected and j gets recovered, so that

$$\begin{aligned}\Pi_{S_iI_j\to S_iR_j} = {}& \langle S_iI_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})\\ &+\langle S_iI_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{iJ_3})\\ &+\langle S_iI_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{iJ_4})\\ &+\cdots+\langle S_iI_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{iJ_3})(1-T_{iJ_4})\\ &+\langle S_iI_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{iJ_4})(1-T_{iJ_5})\\ &+\cdots+\langle S_iI_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{iJ_3})(1-T_{iJ_4})(1-T_{iJ_5})\\ &+\cdots+\langle S_iI_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t\gamma(1-T_{ij})\prod_{h=3}^{m}(1-T_{iJ_h})\end{aligned}\tag{A.3}$$

where the term $\langle S_iI_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})$ takes into account that, even if $J_3,J_4,\dots,J_m$ are not infective, i may still be infected through the link with j, so $\langle S_iI_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t$ is multiplied by the recovery probability γ and the probability that j does not infect i; that is, $(1-T_{ij})$.

Similarly, the term $\Pi_{I_iS_j\to R_iS_j}$ is given by:

$$\begin{aligned}\Pi_{I_iS_j\to R_iS_j} = {}& \langle I_iS_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})\\ &+\langle I_iS_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{jJ_3})\\ &+\langle I_iS_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{jJ_4})\\ &+\cdots+\langle I_iS_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{jJ_3})(1-T_{jJ_4})\\ &+\langle I_iS_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{jJ_4})(1-T_{jJ_5})\\ &+\cdots+\langle I_iS_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma(1-T_{ij})(1-T_{jJ_3})(1-T_{jJ_4})(1-T_{jJ_5})\\ &+\cdots+\langle I_iS_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t\gamma(1-T_{ij})\prod_{h=3}^{m}(1-T_{jJ_h}).\end{aligned}\tag{A.4}$$

For the transition from S_iI_j to I_iI_j to occur, then i has to become infected (eventually through the link with j or one of its neighbors) and j has not to recover, so that:

$$\begin{aligned}\Pi_{S_iI_j\to I_iI_j} &= \langle S_iI_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})]\\ &+\langle S_iI_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{ij_3})]\\ &+\langle S_iI_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{ij_4})]\\ &+\dots+\langle S_iI_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{ij_3})(1-T_{ij_4})]\\ &+\langle S_iI_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{ij_4})(1-T_{ij_5})]\\ &+\dots+\langle S_iI_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{ij_3})(1-T_{ij_4})\\ &\times(1-T_{ij_5})]+\dots+\langle S_iI_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})\prod_{h=3}^{m}(1-T_{ij_h})].\end{aligned} \tag{A.5}$$

Similarly, $\Pi_{I_iS_j\to I_iI_j}$ reads:

$$\begin{aligned}\Pi_{I_iS_j\to I_iI_j} &= \langle I_iS_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})]\\ &+\langle I_iS_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{jJ_3})]\\ &+\langle I_iS_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{jJ_4})]\\ &+\dots+\langle I_iS_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{jJ_3})(1-T_{jJ_4})]\\ &+\langle I_iS_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{jJ_4})(1-T_{jJ_5})]\\ &+\dots+\langle I_iS_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})(1-T_{jJ_3})(1-T_{jJ_4})(1-T_{jJ_5})]\\ &+\dots+\langle I_iS_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t(1-\gamma)[1-(1-T_{ij})\prod_{h=3}^{m}(1-T_{jJ_h})].\end{aligned} \tag{A.6}$$

The transition from S_iI_j to I_iR_j occurs when i becomes infected and j recovers, so that:

$$\begin{aligned}\Pi_{S_iI_j\to I_iR_j} &= \langle S_iI_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})]\\ &+\langle S_iI_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{ij_3})]\\ &+\langle S_iI_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{ij_4})]\\ &+\dots+\langle S_iI_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{ij_3})(1-T_{ij_4})]\\ &+\langle S_iI_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{ij_4})(1-T_{ij_5})]\\ &+\dots+\langle S_iI_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{ij_3})(1-T_{ij_4})(1-T_{ij_5})]\\ &+\dots+\langle S_iI_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t\gamma[1-(1-T_{ij})\prod_{h=3}^{m}(1-T_{ij_h})]\end{aligned} \tag{A.7}$$

and similarly

$$\begin{aligned}\Pi_{I_iS_j\to R_iI_j} &= \langle I_iS_jU_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})]\\ &+\langle I_iS_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{jJ_3})]\\ &+\langle I_iS_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{jJ_4})]\\ &+\dots+\langle I_iS_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{jJ_3})\\ &\times(1-T_{jJ_4})]+\langle I_iS_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{jJ_4})(1-T_{jJ_5})]\\ &+\dots+\langle I_iS_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t\gamma[1-(1-T_{ij})(1-T_{jJ_3})(1-T_{jJ_4})(1-T_{jJ_5})]\\ &+\dots+\langle I_iS_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t\gamma[1-(1-T_{ij})\prod_{h=3}^{m}(1-T_{jJ_h})].\end{aligned} \tag{A.8}$$

The transition from I_iI_j to R_iI_j occurs when j recovers and i does not, so that

$$\Pi_{I_iI_j\to R_iI_j} = \langle I_iI_j\rangle_t\gamma(1-\gamma). \tag{A.9}$$

For a homogeneous recovery rate, the term $\Pi_{I_iI_j\to I_iR_j}$ has the same expression as for $\Pi_{I_iI_j\to R_iI_j}$:

$$\Pi_{I_iI_j\to I_iR_j} = \langle I_iI_j\rangle_t\gamma(1-\gamma). \tag{A.10}$$

The term $\Pi_{R_iS_j\to R_iI_j}$ takes into account that the corresponding transition occurs if j gets the infection:

$$\begin{aligned}\Pi_{R_iS_j\to R_iI_j} &= \langle R_iS_jI_{J_3}U_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_3})]\\ &+\langle R_iS_jU_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_4})]\\ &+\dots+\langle R_iS_jI_{J_3}I_{J_4}U_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_3})(1-T_{jJ_4})]\\ &+\langle R_iS_jU_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_4})(1-T_{jJ_5})]\\ &+\dots+\langle R_iS_jI_{J_3}I_{J_4}I_{J_5}\dots U_{J_m}\rangle_t[1-(1-T_{jJ_3})(1-T_{jJ_4})(1-T_{jJ_5})]\\ &+\dots+\langle R_iS_jI_{J_3}I_{J_4}I_{J_5}\dots I_{J_m}\rangle_t[1-\prod_{h=3}^{m}(1-T_{jJ_h})].\end{aligned} \tag{A.11}$$

The three remaining terms give the probabilities to reach the absorbing state R_iR_j from I_iR_j, R_iI_j or I_iI_j and are given by:

$$\Pi_{I_iR_j\to R_iR_j} = \langle I_iR_j\rangle_t\gamma \tag{A.12}$$

$$\Pi_{R_iI_j\to R_iR_j} = \langle R_iI_j\rangle_t\gamma \tag{A.13}$$

$$\Pi_{I_iI_j\to R_iR_j} = \langle I_iI_j\rangle_t\gamma^2. \tag{A.14}$$

Appendix B. Transition terms for the pair-approximation population model

In this Appendix, the transitions terms appearing in the population model (30) are detailed.

The term $\Pi_{SS\to IS}$ is written by considering that the first node has to be infected by one of its $k-1$ neighbors (the k-th is in the S state) and the other node has not to be infected; that is:

$$\begin{aligned}\Pi_{SS\to IS} &= \langle SSI_1U_2\dots U_{k-1}U_kU_{k+1}\dots U_{2k-2}\rangle_t[1-(1-\tau)](1-\tau)^0\\ &\times\binom{k-1}{0}\binom{k-1}{1}+\dots+\langle SSU_1U_2\dots U_{k-1}I_kU_{k+1}\dots U_{2k-2}\rangle_t\\ &\times[1-(1-\tau)^0](1-\tau)\binom{k-1}{1}\binom{k-1}{0}\\ &+\dots+\langle SSI_1I_2\dots U_{k-1}U_kU_{k+1}\dots U_{2k-2}\rangle_t[1-(1-\tau)^2](1-\tau)^0\\ &\times\binom{k-1}{0}\binom{k-1}{2}+\dots+\langle SSU_1U_2\dots U_{k-1}I_kI_{k+1}\dots U_{2k-2}\rangle_t\\ &\times[1-(1-\tau)^0](1-\tau)^2\binom{k-1}{2}\binom{k-1}{0}\\ &+\dots+\langle SSI_1U_2\dots U_{k-1}I_kU_{k+1}\dots U_{2k-2}\rangle_t[1-(1-\tau)^1](1-\tau)^1\\ &\times\binom{k-1}{1}\binom{k-1}{1}+\dots+\langle SSI_1\dots I_{2k-2}\rangle_t[1-(1-\tau)^{k-1}]\binom{k-1}{k-1}\\ &\times\binom{k-1}{k-1}.\end{aligned} \tag{B.1}$$

By taking into account the closure:

$$\langle SSI_1\dots I_qU_{q+1}\dots U_{2k-2}\rangle = \langle SS\rangle\frac{\langle SI\rangle^q\langle SU\rangle^{2k-2-q}}{\langle S\rangle^{2k-2}} \tag{B.2}$$

and after some manipulation, Eq. (B.1) becomes:

$$\Pi_{SS\to IS} = \langle SS\rangle\sum_{q=1}^{2k-2}\frac{\langle SI\rangle^q\langle SU\rangle^{2k-2-q}}{\langle S\rangle^{2k-2}}\sum_{h=\max(0,q-k+1)}^{\min(q,k-1)}[1-(1-\tau)^{q-h}]\times(1-\tau)^h\binom{k-1}{h}\binom{k-1}{q-h}. \tag{B.3}$$

Similar to Eq. (B.3), the term $\Pi_{SS\to II}$ is written as:

$$\Pi_{SS\to II} = \langle SS\rangle\sum_{q=1}^{2k-2}\frac{\langle SI\rangle^q\langle SU\rangle^{2k-2-q}}{\langle S\rangle^{2k-2}}\sum_{h=\max(0,q-k+1)}^{\min(q,k-1)}[1-(1-\tau)^{q-h}]\times[1-(1-\tau)^h]\binom{k-1}{h}\binom{k-1}{q-h}. \tag{B.4}$$

The term $\Pi_{IS\to RS}$ reads:

$$\begin{aligned}\Pi_{IS\to RS} &= \langle SIUUU\dots U\rangle_t\gamma(1-\tau)+\langle SIIUU\dots U\rangle_t\gamma(1-\tau)^2\binom{k-1}{1}\\ &+\langle SIIIU\dots U\rangle_t\gamma(1-\tau)^3\binom{k-1}{2}+\dots+\langle SIIII\dots I\rangle_t\gamma(1-\tau)^k\binom{k-1}{k-1}.\end{aligned} \tag{B.5}$$

Considering the closure

$$\langle SII_1\ldots I_qU_{q+1}\ldots U_{k-1}\rangle=\langle SI\rangle\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}} \tag{B.6}$$

the term $\Pi_{IS\to RS}$ becomes:

$$\Pi_{SI\to SR}=\langle SI\rangle\sum_{q=0}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}\gamma(1-\tau)^{q+1}\binom{k-1}{q}. \tag{B.7}$$

The term $\Pi_{SI\to II}$ is:

$$\begin{aligned}\Pi_{SI\to II}=&\langle SIUUU\ldots U\rangle_t(1-\gamma)[1-(1-\tau)]+\langle SIIUU\ldots U\rangle_t(1-\gamma)\\&\times[1-(1-\tau)^2]\binom{k-1}{1}+\langle SIIIU\ldots U\rangle_t(1-\gamma)[1-(1-\tau)^3]\binom{k-1}{2}\\&+\cdots+\langle SIIII\ldots I\rangle_t(1-\gamma)[1-(1-\tau)^k]\binom{k-1}{k-1}\end{aligned} \tag{B.8}$$

and with the closure (B.6) it becomes:

$$\Pi_{SI\to II}=\langle SI\rangle\sum_{q=0}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}(1-\gamma)[1-(1-\tau)^{q+1}]\binom{k-1}{q}. \tag{B.9}$$

The term $\Pi_{SI\to IR}$ is given by:

$$\begin{aligned}\Pi_{SI\to IR}=&\langle SIUUU\ldots U\rangle_t\gamma[1-(1-\tau)]+\langle SIIUU\ldots U\rangle_t\gamma[1-(1-\tau)^2]\\&\times\binom{k-1}{1}+\langle SIIIU\ldots U\rangle_t\gamma[1-(1-\tau)^3]\binom{k-1}{2}\\&+\cdots+\langle SIIII\ldots I\rangle_t\gamma[1-(1-\tau)^k]\binom{k-1}{k-1}\end{aligned} \tag{B.10}$$

and considering the closure (B.6) it becomes:

$$\Pi_{SI\to IR}=\langle SI\rangle\sum_{q=0}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}\gamma[1-(1-\tau)^{q+1}]\binom{k-1}{q}. \tag{B.11}$$

The term $\Pi_{II\to RI}$ reads:

$$\Pi_{II\to RI}=\langle II\rangle\gamma(1-\gamma) \tag{B.12}$$

and the term $\Pi_{II\to RR}$ is:

$$\Pi_{II\to RR}=\langle II\rangle\gamma^2. \tag{B.13}$$

The term $\Pi_{RS\to RI}$ reads as:

$$\begin{aligned}\Pi_{RS\to RI}=&\langle RSIUU\ldots U\rangle_t[1-(1-\tau)]\binom{k-1}{1}\\&+\langle RSIIU\ldots U\rangle_t[1-(1-\tau)^2]\binom{k-1}{2}\\&+\cdots+\langle RSIII\ldots I\rangle_t[1-(1-\tau)^k]\binom{k-1}{k-1}.\end{aligned} \tag{B.14}$$

Taking into account the closure:

$$\langle RSI_1\ldots I_qU_{q+1}\ldots U_{k-1}\rangle=\langle RS\rangle\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}} \tag{B.15}$$

$\Pi_{RS\to RI}$ becomes:

$$\Pi_{RS\to RI}=\langle RS\rangle\sum_{q=1}^{k-1}\frac{\langle SI\rangle^q\langle SU\rangle^{k-1-q}}{\langle S\rangle^{k-1}}[1-(1-\tau)^q]\binom{k-1}{q}. \tag{B.16}$$

Finally, the term $\Pi_{RI\to RR}$ is given by:

$$\Pi_{RI\to RR}=\langle RI\rangle\gamma. \tag{B.17}$$

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